

(12) INTERNATIONAL APPLICATION PUBLISHED UNDER THE PATENT COOPERATION TREATY (PCT)

(19) World Intellectual Property
Organization
International Bureau



(43) International Publication Date
29 September 2005 (29.09.2005)

PCT

(10) International Publication Number
WO 2005/091169 A1

(51) International Patent Classification⁷: **G06F 17/30**

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(21) International Application Number:
PCT/EP2005/050891

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(22) International Filing Date: 1 March 2005 (01.03.2005)

(25) Filing Language: English

(26) Publication Language: English

(30) Priority Data:
04100906.9 5 March 2004 (05.03.2004) EP

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(81) Designated States (unless otherwise indicated, for every kind of national protection available): AE, AG, AL, AM, AT, AU, AZ, BA, BB, BG, BR, BW, BY, BZ, CA, CH, CN, CO, CR, CU, CZ, DE, DK, DM, DZ, EC, EE, EG, ES, FI, GB, GD, GE, GH, GM, HR, HU, ID, IL, IN, IS, JP, KE, KG, KP, KR, KZ, LC, LK, LR, LS, LT, LU, LV, MA, MD, MG, MK, MN, MW, MX, MZ, NA, NI, NO, NZ, OM, PG, PH, PL, PT, RO, RU, SC, SD, SE, SG, SK, SL, SM, SY, TJ, TM, TN, TR, TT, TZ, UA, UG, US, UZ, VC, VN, YU, ZA, ZM, ZW.

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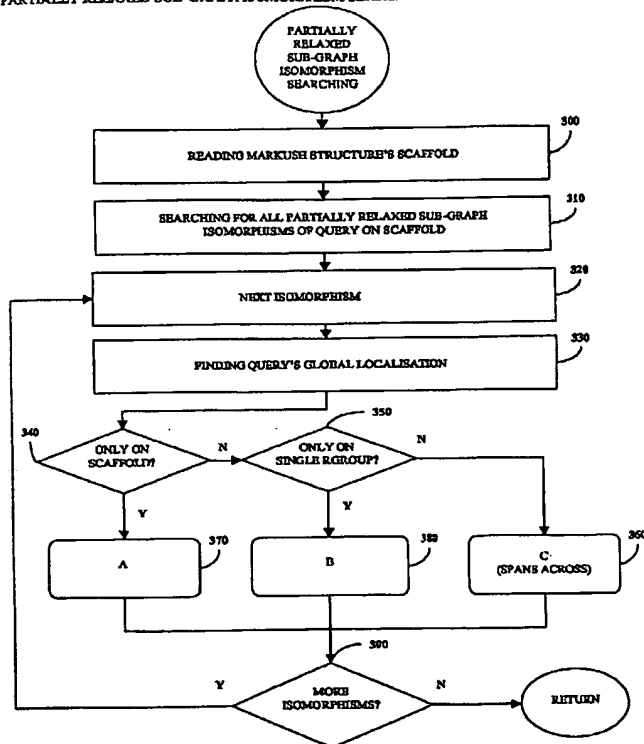
(84) Designated States (unless otherwise indicated, for every kind of regional protection available): ARIPO (BW, GH, GM, KE, LS, MW, MZ, NA, SD, SL, SZ, TZ, UG, ZM, ZW), Eurasian (AM, AZ, BY, KG, KZ, MD, RU, TJ, TM),

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(54) Title: METHOD FOR FAST SUBSTRUCTURE SEARCHING IN NON-ENUMERATED CHEMICAL LIBRARIES

SUBROUTINE:
PARTIALLY RELAXED SUB-GRAPH ISOMORPHISM SEARCHING



(57) Abstract: The present invention relates generally to searching substructures in virtual combinatorial libraries. More precisely, it describes a method of operating a computer for searching substructures in large, non-enumerated virtual combinatorial libraries. Advantageously, the method can return matching products as non-enumerated substructures.

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